

SrPt₃P: two-band single-gap superconductor

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The magnetic penetration depth (λ) as a function of applied magnetic field and temperature in SrPt₃P ($T_c \simeq 8.4$ K) was studied by means of muon-spin rotation (μ SR). The dependence of λ^{-2} on temperature suggests the existence of a single s -wave energy gap with the zero-temperature value $\Delta = 1.58(2)$ meV. At the same time λ was found to be strongly field dependent which is the characteristic feature of the nodal gap and/or multi-gap systems. The multi-gap nature of the superconducting state is further confirmed by observation of an upward curvature of the upper critical field. This apparent contradiction would be resolved with SrPt₃P being a two-band superconductor with equal gaps but different coherence lengths within the two Fermi surface sheets.

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After the discovery of first Fe-based superconductors enormous efforts were made in order to improve their superconducting properties. The intensive search lead to discovery series of new Fe-based materials (see *e.g.* Ref. 1 for review and references therein) and related compounds such as BaNi₂As₂ [2], SrNi₂As₂ [3], SrPt₂As₂ [4], SrPtAs [5], without Fe and relatively low superconducting transition temperatures T_c 's.

Recently, Takayama *et al.* [6] reported the synthesis of a new family of ternary platinum phosphide superconductors with the chemical formula APt₃P (A = Sr, Ca, and La) and T_c 's of 8.4, 6.6 and 1.5 K, respectively. Theoretical studies on the pairing mechanism in these new compounds achieved partially contradicting results [7, 8]. The authors of Ref. 7 performed first-principles calculations and proposed that superconductivity is caused by the proximity to a dynamical charge-density wave instability, and that a strong spin-orbit coupling leads to exotic pairing in at least LaPt₃P. In contrast, the first principal calculations and Migdal-Eliashberg analysis performed by Subedi *et al.* [8] suggest conventional phonon mediated superconductivity. Also experimentally seemingly contradicting results were obtained. Based on the observation of nonlinear temperature behavior of the Hall resistivity, the authors of Ref. 6 suggest multi-band superconductivity in these new compounds. Note that the presence of two bands crossing the Fermi level was indeed confirmed by ab-initio band structure calculations presented in [7–10]. On the other hand the specific heat data of SrPt₃P were found to be well described within a single band, single s -wave gap approach with the zero-temperature gap value of $\Delta = 1.85$ meV [6].

In this paper we report on the results of muon-spin rotation (μ SR) studies of the magnetic penetration depth (λ) as a function of temperature and magnetic field of the novel superconductor SrPt₃P. Below $T \simeq T_c/2$ the superfluid density ($\rho_s \propto \lambda^{-2}$) becomes temperature independent which is consistent with a fully gapped superconducting state. The full temperature dependence of $\rho_s(T)$ is well described within a single s -wave gap scenario with

the zero-temperature gap value $\Delta = 1.58(2)$ meV. On the other hand, λ was found to increase with increasing magnetic field as is observed in multi-band superconductors or superconductors with nodes in the energy gap. The upper critical field demonstrates a pronounced upward curvature thus pointing to a multi-band nature of the superconducting state of SrPt₃P. Our results indicate that SrPt₃P is a two-band superconductor with equal gaps but different coherence length parameters ξ_i within two Fermi surface sheets.

The sample preparation and the magnetization experiments were performed at the ETH-Zürich. Polycrystalline samples of SrPt₃P were prepared using cubic anvil high-pressure and high-temperature technique. Coarse powders of Sr, Pt, and P elements of high purity (99.99%) were weighed according to the stoichiometric ratio 1:3:1, thoroughly grounded, and enclosed in a boron nitride container, which was placed inside a pyrophyllite cube with a graphite heater. All procedures related to the sample preparation were performed in an argon-filled glove box. In a typical run, a pressure of 2 GPa was applied at room temperature. While keeping the pressure constant, the temperature was ramped up in 2 h to the maximum value of 1050 °C, maintained for 20-40 h, and then decreased to room temperature in 1 h. Afterwards, the pressure was released, and the sample was removed. All high-pressure prepared samples demonstrate large diamagnetic response with the superconducting transition temperature of $\simeq 8.4$ K (see the inset in Fig. 1). The powder x-ray diffraction patterns are consistent with those reported in Ref. 6.

Measurements of the upper critical field B_{c2} were performed using a Quantum Design 14 T PPMS. The temperature dependence of B_{c2} was obtained from zero field-cooled magnetization curves [$M_{ZFC}(T)$] measured in constant magnetic fields ranging from 0.3 mT to 4 T (see Fig. 1). For each particular field the corresponding superconducting transition temperature $T_c(B)$ was taken as an intersect of the linearly extrapolated $M_{ZFC}(T)$ curve in the vicinity of T_c with $M_{ZFC} = 0$ line (see the in-

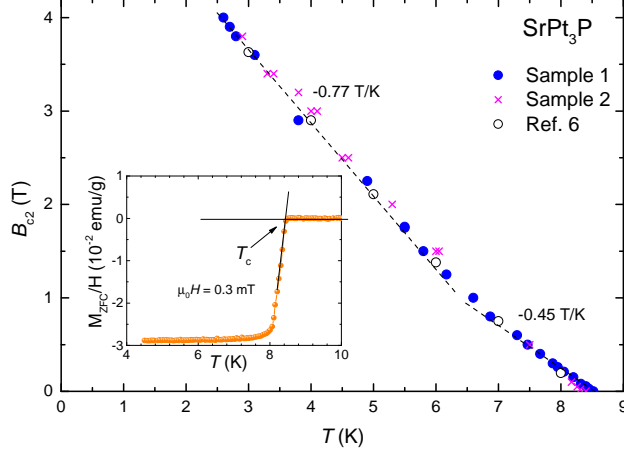


FIG. 1: (Color online) The temperature dependence of the upper critical field B_{c2} of SrPt_3P . The crosses and the circles correspond to two different samples. The solid lines are linear fits of $B_{c2}(T)$ in the vicinity of T_c and for $T \leq 6$ K. Open circles are $B_{c2}(T)$ data points from Ref. 6. The inset shows the temperature dependence of the zero field-cooled magnetization M_{ZFC} measured at $\mu_0 H = 0.3$ mT.

set it Fig. 1). $B_{c2}(T)$ curve exhibits a pronounced upward curvature around $\sim 6 - 6.5$ K. Linear fits of $B_{c2}(T)$ in the vicinity of T_c and for $T \leq 6$ K yield $\text{d}B_{c2}/\text{d}T = -0.45$ and -0.77 T/K, respectively. Open circles correspond to $B_{c2}(T)$ data points from Ref. 6. They are in perfect agreement with our data thus implying that the upturn on $B_{c2}(T)$ reported here is indeed a generic property of SrPt_3P compound. Note that an upward curvature of $B_{c2}(T)$ was also observed previously for a number of materials such as Nb [11, 12], V [11], NbSe₂ [13–15], MgB₂ [16–18], borocarbides and nitrides [19–21], heavy fermion systems [22], various iron-based [23–25] and cuprate superconductors [26, 27] and was often associated with two-band superconductivity.

The temperature and the magnetic field dependence of the magnetic penetration depth λ were obtained from transverse-field (TF) μSR data [28]. The experiments were carried out at the πE1 beam line at the Paul Scherrer Institute (Villigen, Switzerland). The data were analyzed using the free software package MUSRFIT [29]. In a polycrystalline sample the magnetic penetration depth λ can be extracted from the Gaussian muon-spin depolarization rate $\sigma_{sc}(T) \sim \lambda^{-2}$, which reflects the second moment ($\sigma_{sc}^2/\gamma_\mu^2$, γ_μ is the muon gyromagnetic ratio) of the magnetic field distribution due to the flux-line lattice (FLL) in the mixed state [30–32]. The TF- μSR data were analyzed using the asymmetry function:

$$A(t) = A_{sc} \exp[-(\sigma_{sc}^2 + \sigma_n^2)t^2/2] \cos(\gamma_\mu B_{sc}t + \phi) + A_b \exp(-\sigma_b^2 t^2/2) \cos(\gamma_\mu B_b t + \phi) \quad (1)$$

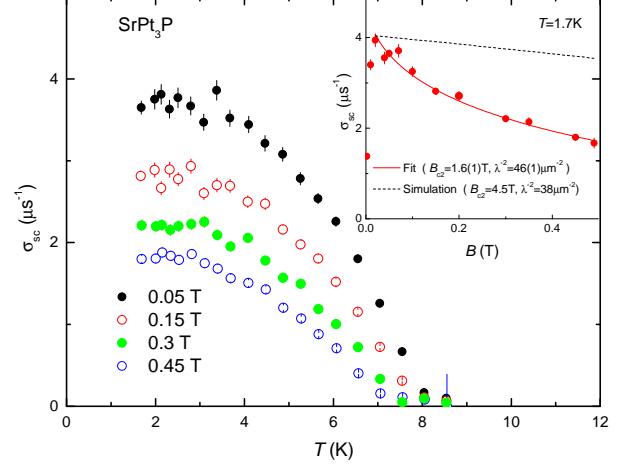


FIG. 2: (Color online) The temperature dependence of the depolarization rate σ_{sc} caused by formation of FLL in SrPt_3P in fields of 0.05, 0.15, 0.3, and 0.45 T. The inset shows the dependence of σ_{sc} on the applied field B at $T = 1.7$ K. The red solid line is the fit of Eq. (2) to $\sigma_{sc}(B)$ data with $\lambda^{-2} = 46(1) \mu\text{m}^{-2}$, $B_{c2} = 1.6(1)$ T. The dashed black line represent $\sigma_{sc}(B)$ as expected for $\lambda^{-2} = 38(1) \mu\text{m}^{-2}$ and $B_{c2} = 4.5$ T obtained in magnetization experiments.

The first term of Eq. (1) represents the response of the superconducting part of the sample. Here A_{sc} denotes the initial asymmetry; σ_{sc} is the Gaussian relaxation rate due to the FLL; σ_n is the contribution to the field distribution arising from the nuclear moment and which is found to be temperature independent, in agreement with the ZF results (not shown); B_{int} is the internal magnetic field sensed by the muons and ϕ is the initial phase of the muon-spin ensemble. The second term with the initial asymmetry A_b , small $\sigma_b < 0.3 \mu\text{s}^{-1}$ and B_b close to the applied field corresponds to the background muons stopping in the cryostat and in nonsuperconducting parts of the sample.

Figure 2 shows the temperature dependence of σ_{sc} in four different fields 0.05, 0.15, 0.3, and 0.45 T. As expected, σ_{sc} is zero in the paramagnetic state and starts to increase below the corresponding $T_c(B)$. Upon lowering T , σ_{sc} increases gradually reflecting the decrease of the penetration depth λ or, correspondingly, the increase of the superfluid density $\rho_s \propto \lambda^{-2}$. The overall decrease of σ_{sc} with increasing applied field is partially caused by the decreased width of the internal field distribution upon approaching B_{c2} . In order to quantify such an effect, one can make use of the numerical Ginzburg-Landau model, developed by Brandt [33]. This model predicts the magnetic field dependence of the second moment of the magnetic field distribution, *i.e.* μSR depolarization rate:

$$\sigma_{sc}[\mu\text{s}^{-1}] = 4.83 \cdot 10^4 (1 - B/B_{c2}) \times$$

$$\times [1 + 1.21(1 - \sqrt{B/B_{c2}})^3] \lambda^{-2} [\text{nm}^{-2}] (2)$$

The insert of Fig. 2 shows the evolution of σ_{sc} at $T = 1.7$ K as a function of the applied magnetic field B . Each data point was obtained after cooling the sample in the corresponding field from above T_c to 1.7 K. Under the assumption of field independent λ the dependence of σ_{sc} on B was analyzed by means of Eq. (2) using the values of the upper critical field B_{c2} as obtained in magnetization experiments [$B_{c2}(1.7 \text{ K}) \simeq 4.5 \text{ T}$, see Fig. 1]. It is clear from the inset of Fig. 3 that the theoretical $\sigma(B)$ is not in agreement with the data. If B_{c2} is kept as a free parameter in the analysis, the fit yields $B_{c2} = 1.6(1) \text{ T}$ which is clearly inconsistent with the magnetization data. Therefore one has to conclude that the field independence of λ , which was implicitly assumed in Eq.(2), is not valid (the discussion on field dependence of λ comes later in the paper). The low-temperature value of λ at $B = 0$ [$\lambda(0, B = 0)$] could be estimated by extrapolating two theory lines shown in the inset of Fig. 2 to $B = 0$. This results in $\lambda(0, B = 0) = 155 \pm 10 \text{ nm}$.

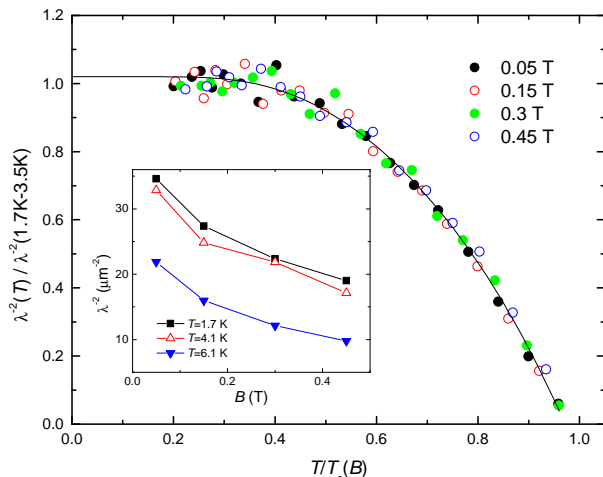


FIG. 3: (Color online) $\lambda^{-2}(T)$ normalized to its value averaged over the temperature range 1.7 – 3.5 K as a function of $T/T_c(B)$. The solid line is the fit by using the weak-coupling BCS model (see Eq. 3). The inset shows the dependence of λ^{-2} on the applied field at $T = 1.7, 4.1$ and 6.1 K .

The temperature dependences of λ^{-2} for $\mu_0 H = 0.05, 0.15, 0.3$, and 0.45 T was obtained from measured $\sigma_{sc}(T)$'s and $B_{c2}(T)$ by using Eq. (2). Figure 3 shows $\lambda^{-2}(T)$ normalized to its value averaged over the temperature range 1.7 – 3.5 K as a function of $T/T_c(B)$. All data curves merge into the single line. The inset of Fig. 3 shows the field dependence of λ^{-2} for $T = 1.7, 4.1$ and 6.1 K .

As a first step we are going to discuss the temperature dependence of λ^{-2} . It is seen that below approximately

one half of T_c , λ^{-2} is temperature independent. The solid line in Fig. 3 represents fit with the weak-coupling BCS model [34]:

$$\frac{\lambda^{-2}(T)}{\lambda^{-2}(0)} = \frac{\rho_s(T)}{\rho_s(0)} = 1 + 2 \int_{\Delta(T)}^{\infty} \left(\frac{\partial f}{\partial E} \right) \frac{E dE}{\sqrt{E^2 - \Delta(T)^2}}. \quad (3)$$

Here $\lambda^{-2}(0)$ and $\rho_s(0)$ are the zero-temperature values of the magnetic penetration depth and the superfluid density, respectively, and $f = [1 + \exp(E/k_B T)]^{-1}$ is the Fermi function. The temperature dependence of the gap is approximated by $\Delta(T)/\Delta(0) = \tanh\{1.82[1.018(T_c/T - 1)]^{0.51}\}$ [35], where $\Delta(0)$ is the maximum gap value at $T = 0$. The fit results in $\Delta(0, B)/k_B T_c(B) = 4.35(4)$, $\lambda^{-2}(T)/\lambda^{-2}(1.7 - 3.5 \text{ K}) = 1.021(6)$, and $T/T_c(B) = 0.972(3)$. For $T_c(B = 0) \simeq 8.4 \text{ K}$ (see Fig. 1) we get $\Delta(T = 0, B = 0) = 1.58(2) \text{ meV}$. Note that this value of the superconducting gap is close to $\Delta = 1.85 \text{ meV}$ obtained from zero-field specific heat data by Takayama *et al.* [6].

It is noteworthy that there is no need to introduce more than one gap parameter or to consider more complicated gap symmetry in order to satisfactorily describe $\lambda^{-2}(T)$ data. A fit using two superfluid density components with s -wave gaps Δ_1 and Δ_2 : $\lambda^{-2}(T) = \lambda_1^{-2}(T, \Delta_1) + \lambda_2^{-2}(T, \Delta_2)$, as well as a fit using an anisotropic s -wave gap function result in higher χ^2 than obtained for the simple one gap s -wave model described above. From the analysis of $\lambda^{-2}(T)$ data alone one could therefore conclude that SrPt₃P is a single band s -wave superconductor. Note that the similar conclusion was reached by Takayama *et al.* [6] based on specific heat data. In the following we will suggest that this was a premature conclusion obtained without considering the field dependence of λ .

As follows from the inset in Fig. 3, the field increase from 0.05 up to 0.45 T leads to decrease of λ^{-2} by almost a factor of 2. In a single band s -wave superconductors λ is independent on the magnetic field [31, 35–37]. A dependence of λ on B is expected for superconductors containing nodes in the energy gap or/and multi-gap superconductors [32, 36, 38–40]. In the later case the superfluid density within one series of bands is expected to be suppressed faster by magnetic field than within the others [39, 40].

The single s -wave gap behavior of $\lambda^{-2}(T)$ (see Fig. 3 and the discussion above) and the multi-band features following after the upper critical field B_{c2} and $\lambda^{-2}(B)$ measurements (Fig. 1 and the inset on Fig. 3) allow us to assume that SrPt₃P is a *two-band* superconductor with energy gaps being *equal* within both bands.

Within a two-gap model the deviation from the simple field independence of λ as well as the appearance of upward curvature of the upper critical field could reflect the occurrence of two distinct coherence lengths ξ_1 and ξ_2 for two bands (associated to the corresponding upper critical field values $B_{c2,i} = \phi_0/2\pi\xi_i^2$) [39–44]. For BCS

superconductors the zero-temperature coherence length obeys the relation $\xi \propto \langle v_F \rangle / \Delta$, ($\langle v_F \rangle$ is the averaged value of the Fermi velocity). One could assume, therefore that in SrPt₃P the difference between ξ_1 and ξ_2 could be caused by the different Fermi velocities ($\langle v_{F,1} \rangle \neq \langle v_{F,2} \rangle$), while gaps remain the same ($\Delta_1 = \Delta_2$).

The statement about different $\langle v_F \rangle$'s in two Fermi surface sheets of SrPt₃P is fully confirmed by the calculated band structure [7–10]. According to Refs. 7–10 there are two bands crossing the Fermi level having significantly different v_F 's. The ratio of v_F 's is, *e.g.*, $\simeq 2$ along $\Gamma - X$ and $\sim 3 - 4$ along $\Gamma - Z$ directions of the Brillouin zone. It is worth to note that different Fermi velocities on the different superconducting bands suppose to be a common feature of multi-band superconductors as *e.g.* MgB₂ [45–47], borocarbides [20, 47], Fe-based superconductors [48, 49] *etc.*

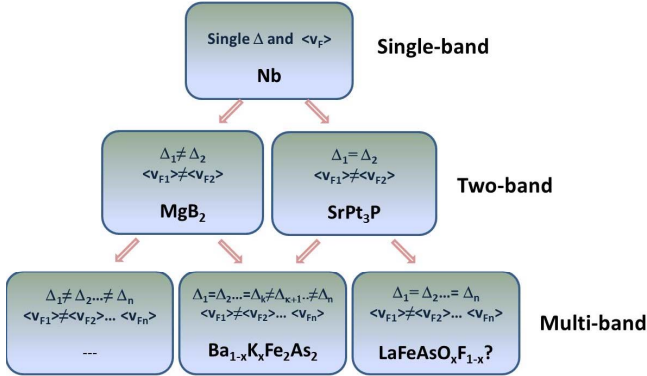


FIG. 4: (Color online) Schematic diagram representing relations between the various types of a single-band, two-band and multi-band superconductors.

Note SrPt₃P studied here is different from the most famous two-band superconductor MgB₂. In SrPt₃P the charge carriers in both bands suppose to be almost equally coupled to the phonons. Indeed, according to the band structure calculations of Nekrasov *et al.* [9] the carriers in two bands correspond to the relatively *similar* $pd\pi$ antibonding states of Pt(I)-P and Pt(II)-P ions, and are coupled to the *same* low-lying phonon modes confined on the *ab* plane. In MgB₂ only the σ band carriers are coupled strongly to the so called E_{2g} phonons, while the coupling of both, the σ and the π , bands to the harmonic B_{1g} , A_{2u} , and E_{1u} phonons is negligible [50]. We may conclude, therefore, that MgB₂ and SrPt₃P correspond to two limiting cases of two-band superconductivity with the energy gaps being nonequal ($\Delta_1 \neq \Delta_2$, as in MgB₂) and equal ($\Delta_1 = \Delta_2$, as in SrPt₃P). At the same time SrPt₃P remains the "true" two-band superconductor since, due to nonequal Fermi velocities ($\langle v_{F,1} \rangle \neq \langle v_{F,2} \rangle$), the carriers in various bands "respond" differently to the magnetic field (as shown here

based on $B_{c2}(T)$ and $\lambda(B)$ studies and by Takayama *et al.* [6] based on the observation of nonlinear temperature behavior of the Hall resistivity).

By following the above presented arguments we propose a schematic diagram describing relations between the single-, two-, and the multi-band superconductivity (see Fig. 4). The single-band superconductor has one gap and one averaged over the Fermi surface Fermi velocity ($\langle v_F \rangle$). There are two type of two-band superconductors with energy gaps being equal ($\Delta_1 = \Delta_2$) and nonequal ($\Delta_1 \neq \Delta_2$). Both of these types are characterized, however, by nonequal $\langle v_F \rangle$'s. The "transition" from the two- to the multi-band superconductivity may occur by three different routes. (i) All gaps in all bands crossing the Fermi level are equal ($\Delta_1 = \Delta_2 \dots = \Delta_n$). This is probably the case for the optimally doped LaFeAsO_{0.9}F_{0.1} having five Fermi surfaces (as most other Fe-based superconductors, see *e.g.* Ref. 1 and references therein). As shown by Luetkens *et al.* [51] the temperature evolution of the superfluid density of LaFeAsO_{0.9}F_{0.1} is well described within the single *s*-wave gap approach, while λ^{-2} depends strongly on the magnetic field. It should be noted, however that the presence of two distinct gaps in LaFeAsO_{0.9}F_{0.1} were reported by Gonnelli *et al.* [52] based on the result of point contact Andreev reflection experiment. (ii) Gaps in some Fermi sheets are equal but in others are not ($\Delta_1 = \Delta_2 \dots = \Delta_k \neq \Delta_{k+1} \dots \neq \Delta_n$). A good example is the optimally doped Ba_{1-x}K_xFe₂As₂ where three gaps are equal ($\simeq 9$ meV) while the last gap was found to be of approximately eight times smaller ($\simeq 1.1$ meV) [48, 53]. (iii) Gaps in all the Fermi sheets are different ($\Delta_1 \neq \Delta_2 \dots \neq \Delta_n$).

To summaries, the temperature and the magnetic field dependence of the magnetic penetration depth λ in SrPt₃P superconductor ($T_c \simeq 8.4$ K) were studied by means of muon-spin rotation. Below $T \simeq T_c/2$ the superfluid density $\rho_s \propto \lambda^{-2}$ is temperature independent which is consistent with a fully gapped superconducting state. The full $\rho_s(T)$ is well described within the single *s*-wave gap scenario with the zero-temperature gap value $\Delta = 1.58(2)$ meV. At the same time λ was found to be strongly field dependent which is the characteristic feature of the nodal gap and/or multi-band systems. The multi-band nature of the superconducting state in SrPt₃P was further confirmed by observation of an upward curvature of the upper critical field. To conclude, all above presented results show SrPt₃P to be a two-band superconductor with the equal gaps but different coherence lengths ξ_i associated with the two Fermi surface sheets.

This work was performed at the Swiss Muon Source (μ S), Paul Scherrer Institute (PSI, Switzerland).

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